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Silicon adatom chains and one-dimensionally confined electrons on 4H-SiC($1\bar{1}02$): The (2×1) reconstruction

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ABSTRACT

The electronic and atomic structure of the 4H-SiC($1\bar{1}02$) – (2×1) surface was investigated. Photoemission data indicate that the surface contains about 2 Si layers on top of the bulk layers. Scanning tunneling microscopy images show that these adlayers are terminated by an ordered array of adatom chains separated by the unit cell size. An electronic surface state located at a binding energy of 0.8 eV shows one-dimensional confinement with dispersion only along the chains. Based on the experimental observations, a tentative (2×1) surface model is derived with the surface terminated by alternating chains of Si adatoms and Si dimers in between.

1. Introduction

Silicon carbide is a wide band gap semiconductor suitable for devices operable at high temperature, high voltage, high frequency and high power. Numerous studies of the SiC basal plane surfaces have been carried out [1], motivated in part by material problems in connection with industrial device production. However, in recent years SiC surfaces have also attracted a fundamental interest in view of their electronic properties. A remarkable property of SiC surfaces is the strong Coulomb repulsion between electrons in the same dangling bond orbital leading to electron correlation effects on many reconstruction phases [2]. This would be particularly interesting for one-dimensional systems as suggested recently [3,4] which could be achieved with strongly anisotropic atomic arrangements. On the bio-compatible and semiconducting material SiC this opens up possibilities for bio-sensors and nano-devices. Quite promising for one-dimensionality are non-basal plane surfaces since they directly exhibit the long period of the SiC bulk polytype stacking in the direction of the *c*-axis. Specifically in a plane orientation situated diagonally in the bulk unit cell of 4H-SiC this stacking sequence entails an anisotropic bulk truncated surface structure [5]. The (1×1) unit cell of a bulk like 4H-SiC($1\bar{1}02$) surface contains two regions of different bond configuration, corresponding to alternating stripes of hexagonal type, i.e (0001) basal plane, and cubic type surface atom configuration [5]. By using Si deposition and annealing in ultra-high vacuum (UHV) three ordered reconstructions of varying surface composition can be prepared [6], namely a Si rich (2×1) phase, a $c(2 \times 2)$ phase of nearly bulk-like stoichiometry which has been analysed recently [7] and a (1×1) phase that is C rich due to high temperature annealing. The present paper reports the investigation of the (2×1) reconstruction on this surface which indeed reveals a one-dimensional nature of the atomic and electronic structure.

2. Experimental

In this investigation, we performed a combination of experiments using core level photoemission (PES) and angle resolved photoemission (ARPES) at the MAX synchrotron radiation laboratory (Lund, Sweden), scanning tunneling microscopy (STM) and

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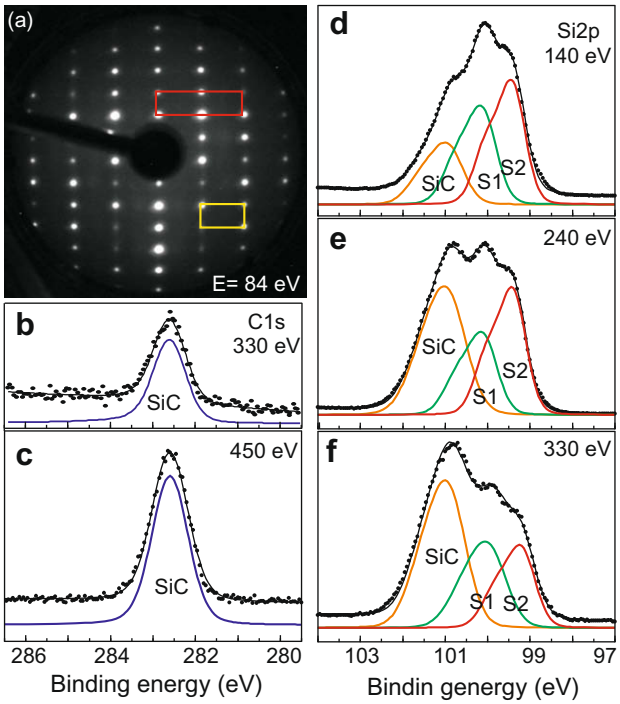

Fig. 1. (a) LEED pattern of the (2×1) reconstructed 4H-SiC$(1\bar{1}02)$ surface acquired at 84 eV electron energy, with the red (1×1) and yellow (2×1) unit cells indicated. (b) and (c) C1s core level spectra recorded at photon energies of 330 and 450 eV. (d)–(f) Si2p spectra recorded at a photon energy of 140, 240 and 330 eV, respectively. The solid curves through the data points represents the results of the curve fits with the components shown underneath [11]. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article).

low-energy electron diffraction (LEED). The core level experiments were carried out in the endstation of beam line I311 [8].[2] The ARPES investigations of the valence band (VB) were performed at beam line 33 with a goniometer based angle resolving electron analyser [9].[3] For the dispersion measurements along different directions of the surface Brillouin zone (BZ), the sample was oriented with LEED so that the angle (i.e. $\mathbf{k}_{\parallel}$) was always scanned in the horizontal plane. The STM studies were performed in a home-built ultra-high vacuum (UHV) chamber equipped with a Besocke type STM [10].

Ex situ hydrogen etched 4H-SiC$(1\bar{1}02)$ samples were loaded into the UHV chamber and prepared by heating during simultaneous Si deposition. In this way, by applying different temperatures, several ordered reconstruction phases with different surface composition can be produced [6]. The (2×1) reconstructed phase discussed in the present paper develops at temperatures between 830 °C and 900 °C with a sharp LEED pattern as shown in Fig. 1a.

3. Structural results

The 4H-SiC$(1\bar{1}02) - (2 \times 1)$ surface is of Si rich composition as indicated by the core level spectra shown in Fig. 1b–f. While the C1s spectrum even at the highest surface sensitivity (panel b) contains only a bulk SiC component at a binding energy of 282.6 eV,

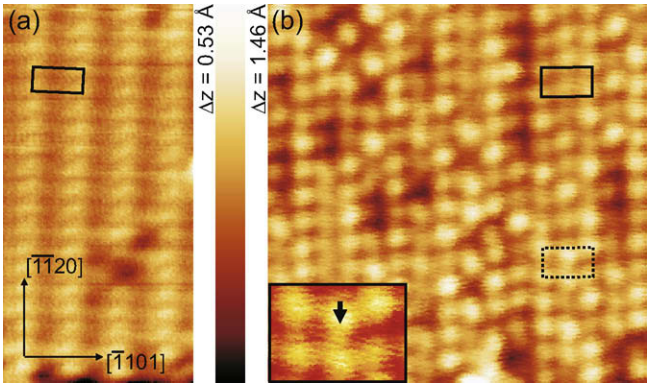

Fig. 2. STM micrographs of the (2×1) reconstruction on 4H-SiC$(1\bar{1}02)$ (a) taken with −2 V tip bias (empty state) and 0.3 nA tunneling current. The surface unit cell and the low Miller index crystal directions are indicated (5 nm × 10 nm). (b) Filled state STM image (9 nm × 9 nm) with +2 V tip bias. On the right side domains with a different position of the second protrusion are indicated by solid and dashed unit cells, the inset depicts its lateral shift. The full *z*-scale as indicated by the scale bar in between is 0.53 Å for (a) and 1.46 Å for (b), respectively.

for the Si2p level two prominent surface shifted components (labeled S1 and S2) besides bulk SiC are obtained from a line shape analysis [11].[4] This shows that the reconstruction is entirely restricted to the Si adlayers. The S1 and S2 components have shifts of −0.9 and −1.6 eV relative to the bulk SiC peak which in turn is located at a binding energy of 100.9 eV. Differences in the relative intensity ratio of the S1 and S2 components compared to the bulk component are clearly visible at different photon energies as shown in Fig. 1d–f. The S2/bulk ratio shows the largest variation with photon energy and the S2 component is strongest for the lowest photon energy selected (140 eV). Accordingly, S2 corresponds to Si adatoms located in the outermost surface layer. The S1/bulk ratio shows a smaller variation with photon energy, which indicates that S1 originates from Si atoms located at an interface between the bulk and the outermost Si atoms (S2). This assignment is qualitatively consistent with the binding energy shifts of the two components when compared to earlier reports [12,13] of surface core level shifts for the SiC(0001)-(3×3) surface reconstruction [14]. By analyzing the peak attenuation with an electron mean free path model, the thickness of the topmost Si layers (S1 and S2 components) can be estimated to about 3 Å.

An empty state STM image of the surface shows a single protrusion per (2×1) unit cell as indicated by the rectangle in Fig. 2a. The protrusions form rows with a period within the row of 6 Å and obviously correspond to atomic chains of Si adatoms. The chains are separated by the surface unit cell length (1.2 nm) in $[\bar{1}101]$ direction and form a regular pattern with the periodicity in this direction corresponding to the bilayer stacking in the 4H-SiC polytype as it is projected onto the $(1\bar{1}02)$ surface. Occasional defects visible in the image are concentrated in the channels between the adatom rows while the rows are mostly well ordered. In Fig. 2b an STM image of the filled states is displayed which reveals further details of the unit cell. Here again the well ordered rows can be identified, but an additional high charge density is resolved in the middle between the adatom rows. In average its *z*-position appears to be slightly below that of the adatom rows in most cases, although a variation is observed that indicates some disorder

[2] The Si2p and C1s core levels were measured at photon energies between 140 and 450 eV with a total energy resolution ranging from 20 to 100 meV in normal emission, an angular acceptance of ±8° and a photon incidence angle of 55°. Binding energies were referenced to the Fermi level determined from a Ta foil mounted on the sample holder.

[3] The angular resolution was set to ±2°, the total energy resolution to less than 120 meV. Photon energies were used from 14 to 95 eV with an incidence angle of 45°.

[4] For the fit of the C1s peak, a Lorentzian width of 0.18 was selected. The best fit was obtained with a Gaussian width of 0.9 eV for the bulk SiC component. For the Si2p levels a spin orbit splitting of 0.61 eV, a branching ratio of 0.50 and a Lorentzian width of 0.07 were used. The asymmetry parameter was set to zero for both core levels. Best fits for the Si2p level were obtained for Gaussian widths of 0.9 eV for the bulk SiC component and 0.8 and 0.7 eV for the S1 and S2 components, respectively.